

AN ALGORITHM FOR DETECTING INTRINSICALLY KNOTTED GRAPHS

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ABSTRACT. We describe an algorithm that recognizes some (perhaps all) intrinsically knotted (IK) graphs, and can help find knotless embeddings for graphs that are not IK. The algorithm, implemented as a Mathematica program, has already been used in [6] to greatly expand the list of known minor minimal IK graphs, and to find knotless embeddings for some graphs that had previously resisted attempts to classify them as IK or non-IK.

1. INTRODUCTION

All graphs in the paper are finite. A graph is **intrinsically knotted** (IK) if every embedding of it in S^3 contains a nontrivial knot. In the early 1980s Conway and Gordon [1] showed that K_7 , the complete graph on seven vertices, is IK. A graph H is a **minor** of another graph G if H can be obtained from a subgraph of G by contracting some edges. A graph G with a given property is said to be **minor minimal** with respect to that property if no proper minor of G has that property. Robertson and Seymour's Graph Minor Theorem [9] says that in any infinite set of graphs, at least one is a minor of another. It follows that for any property whatsoever, there are only finitely many graphs that are minor minimal with respect to that property. In particular, there are only finitely many minor minimal IK graphs. It is well known and easy to show that G is IK iff G contains a minor minimal IK graph as a minor. Hence, if we had a list of all minor minimal IK graphs, then we could determine whether or not any given graph G is IK by testing whether G contains one of the graphs in this list as a minor. But, for about the past three decades, finding such a list has remained an open problem. Our algorithm, which does not rely on having such a list available, can recognize some (perhaps all) IK graphs.

Prior to this algorithm, finding new minor minimal IK graphs was quite difficult. Initially, the only known minor minimal IK graphs were K_7 and the thirteen graphs obtained from it by ∇Y moves ([1], [5]). About two decades later the list expanded to include $K_{3,3,1,1}$ plus the 25 graphs obtained from it by ∇Y moves ([2], [5]). And a few years later Foisy [3] discovered one more minor minimal IK graph. These 41 graphs were the only minor minimal IK graphs known before this algorithm. With the aid of our algorithm, Goldberg, Mattman, and Naimi [6] have found over 1600 new IK graphs, over 200 of which have been proven to be minor minimal IK. The algorithm has also helped us find knotless embeddings for some graphs that

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had previously resisted attempts to determine whether or not they are IK. For the graphs we worked on, our program typically took from less than a minute to less than a day to run on an average personal computer. A large portion of the time is usually spent on just finding all the cycles in the given graph; and a good predictor of computation time seems to be the number of edges in the graph. We found that for some graphs with about 30 or more edges, the program could take days (or much longer) to run.

Before describing our algorithm, we need to introduce some more notation and terminology. The linking number of two disjoint cycles C_1 and C_2 in a spatial graph (i.e., a graph embedded in S^3) is denoted by $\text{lk}(C_1, C_2)$. If K is a knot in S^3 , $a_2(K)$ denotes the second coefficient of the Conway polynomial of K . The graph depicted in Figure 1 is denoted by D_4 . It has four vertices and eight edges. The cycles C_1, \dots, C_4 are always assumed to be labeled in the order shown, so that $C_1 \cap C_3 = \emptyset$ and $C_2 \cap C_4 = \emptyset$.

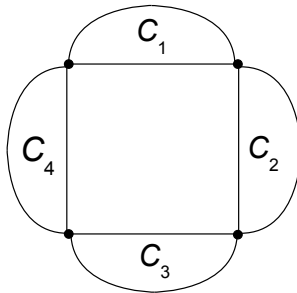


FIGURE 1. The graph D_4 .

If D_4 is embedded in S^3 in such a way that $\text{lk}(C_1, C_3) \neq 0$ and $\text{lk}(C_2, C_4) \neq 0$, then we say it is a **double-linked** D_4 . If these linking numbers are both nonzero in \mathbb{Z}_2 , we say the embedded D_4 is **double-linked in \mathbb{Z}_2** . The following lemma was proved by Taniyama and Yasuhara [11] in \mathbb{Z} and by Foisy [2] in \mathbb{Z}_2 .

Lemma. (D_4 -Lemma, [2], [11]) *Every double-linked D_4 (in \mathbb{Z} or \mathbb{Z}_2) contains a knot K such that $a_2(K) \neq 0$ (in \mathbb{Z} or \mathbb{Z}_2 , respectively).*

A **D_4 -less embedding** (in \mathbb{Z} or \mathbb{Z}_2) of a graph is an embedding that contains no double-linked D_4 (in \mathbb{Z} or \mathbb{Z}_2) as a minor (note: a minor H of an embedded graph G can in a natural way be given an embedding that is “derived” from the given embedding of G). Since any knot K with $a_2(K) \neq 0$ is nontrivial, an immediate corollary of the above lemma is:

Corollary. *If a graph has no D_4 -less embedding (in \mathbb{Z} or \mathbb{Z}_2), then it is IK.*

Given any graph G , our algorithm searches for a D_4 -less embedding of G in \mathbb{Z} or \mathbb{Z}_2 . If it finds one, it reports this embedding, which, as we’ll explain later, may help us find a knotless embedding for G . If the algorithm determines that there is no such embedding, we conclude by the above corollary that G is IK.

Using this algorithm, Goldberg, Mattman, and Naimi [6] have found over 1600 new IK graphs, most of which seem to be minor minimal IK, and 222 of which were “manually” verified in [6] to be minor minimal IK.

Foisy [4] has asked the following question (which is the converse of the above corollary):

Question [4]: Does every graph that has a D_4 -less embedding (in \mathbb{Z} or \mathbb{Z}_2) have a knotless embedding?

If the answer to this question is affirmative, then in fact our algorithm (without the third shortcut described in Section 3) *always* decides whether or not a graph is IK. In [6], in every instance that the algorithm found a D_4 -less embedding for a graph G , whenever the authors tried to manually find a knotless embedding for G , they succeeded.

Let's define a spatial graph Γ to be an a_2 -**less embedding** (in \mathbb{Z} or \mathbb{Z}_2) if for every knot $K \subset \Gamma$, $a_2(K) = 0$ (in \mathbb{Z} or \mathbb{Z}_2). It is then natural to ask:

- (1) Does every graph that has a D_4 -less embedding (in \mathbb{Z} or \mathbb{Z}_2) have an a_2 -less embedding (in \mathbb{Z} or \mathbb{Z}_2)?
- (2) Does every graph that has an a_2 -less embedding (in \mathbb{Z} or \mathbb{Z}_2) have a knotless embedding?

The algorithm sets up systems of linear equations involving linking numbers of certain pairs of cycles in G in terms of variables representing the number of crossings between pairs of edges. These equations are such that there is a solution to at least one of the systems of equations if and only if G has a D_4 -less embedding. The number of equations the algorithm needs to solve grows exponentially with the size of G . So it was necessary to find various shortcuts to speed up the algorithm. We describe the algorithm in Section 2, the shortcuts in Section 3, and the proofs in Section 4.

Using similar techniques, we have also written a Mathematica program that determines whether or not any given graph is intrinsically linked (IL), i.e., every embedding of it in S^3 contains a nontrivial link. The algorithm relies on the work of Robertson, Seymour, and Thomas [10], which implies that if a spatial graph contains a nontrivial link, then it contains a 2-component link with odd linking number. Note that, by [10], an algorithm for recognizing IL graphs was already known: simply check whether the given graph contains as a minor one of the seven graphs in the Petersen Family — which, by [8], can be done in polynomial time (though the polynomial has very large coefficients). And in [12], van der Holst gives polynomial-time algorithms to find an embedding of a graph with all linking numbers zero, given that such an embedding exists. Our algorithm is not polynomial time (since the number of cycles can grow exponentially with the number of edges); but, in practice, we found it satisfactorily fast and practical for the graphs that we tried out: for graphs with 28 or fewer edges, the program usually took from about a few seconds to a couple of hours to run on a typical personal computer in 2009. More specifically, the computer program was run on at least the following graphs listed in [6] and [7]: all graphs in the K_7 , $K_{3,3,1,1}$, and $E_9 + e$ families (188, all together); the 25 parentless (“top level”) graphs and a few dozen other graphs in the $G_{9,28}$ family; and the graph $G_{14,25}$ plus a few more in its family.

2. THE ALGORITHM

A **quad** in a graph G is an ordered 4-tuple (C_1, C_2, C_3, C_4) of distinct cycles in G such that $C_1 \cap C_3 = C_2 \cap C_4 = \emptyset$, and for each $i \in \{1, 2, 3, 4\}$, either $C_i \cap C_{i+1}$ is nonempty and connected (where an index of $4 + 1$ is to be interpreted as 1), or

$C_i \cap C_{i+1} = \emptyset$ and there exists a path p_i in G with one endpoint in C_i and the other in C_{i+1} , satisfying the following conditions:

- (1) Each path p_i is disjoint from C_j for $j \notin \{i, i+1\}$.
- (2) The interior of each p_i is disjoint from C_i and C_{i+1} .
- (3) Any two distinct paths p_i and p_j are disjoint.

Furthermore, for each i where $C_i \cap C_{i+1}$ is nonempty and connected, we let p_i consist of an arbitrary vertex in $C_i \cap C_{i+1}$. (We do this so that p_i is defined for every i , allowing for more uniformity in notation). We say p_1, \dots, p_4 are **connecting paths** for the given quad. Figure 2 shows an example of this. It is easy to see that for any quad (C_1, C_2, C_3, C_4) together with connecting paths p_i , their union $(\bigcup_i C_i) \cup (\bigcup_i p_i)$ contains D_4 as a minor.

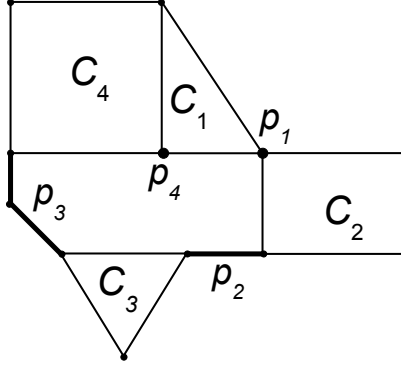


FIGURE 2. An example of a quad, with thickened connecting paths.

We say a quad (C_1, C_2, C_3, C_4) in a spatial graph Γ is **double-linked** (in \mathbb{Z} or \mathbb{Z}_2) if $\text{lk}(C_1, C_3) \neq 0$ and $\text{lk}(C_2, C_4) \neq 0$ (in \mathbb{Z} or \mathbb{Z}_2 , respectively).

It is easy to see that a spatial graph that contains a double-linked quad contains a double-linked D_4 as a minor. Lemma 2, which we will prove later, says that the converse of this is also true, i.e.,

If a spatial graph Γ contains a double-linked D_4 (in \mathbb{Z} or \mathbb{Z}_2) as a minor, then it contains a double-linked quad (in \mathbb{Z} or \mathbb{Z}_2 , respectively).

Hence an embedding Γ of a graph G is a D_4 -less embedding iff for every quad (C_1, C_2, C_3, C_4) in Γ , $\text{lk}(C_1, C_3) = 0$ or $\text{lk}(C_2, C_4) = 0$. We translate this into systems of linear equations as follows. Let Γ_0 be a fixed arbitrary embedding of G . Then any embedding Γ of G can be obtained from Γ_0 by a sequence of crossing changes together with ambient isotopy in S^3 . Let e_1, \dots, e_n denote the edges of G . For each pair of nonadjacent edges e_i and e_j , let x_{ij} denote the total number of crossing changes between e_i and e_j in the given sequence of crossing changes that takes Γ_0 to Γ . (Crossing changes between adjacent edges are ignored since they do not affect any linking numbers.) Note that x_{ij} is the *algebraic* sum of the crossing changes between e_i and e_j , where we give each edge an arbitrary fixed orientation, and associate a $+1$ to each crossing change that changes a left-handed crossing into

a right-handed one, and a -1 for the opposite case (see Figure 3). (Alternatively, one can think of each crossing change as adding a full positive or negative twist between the two edges.)

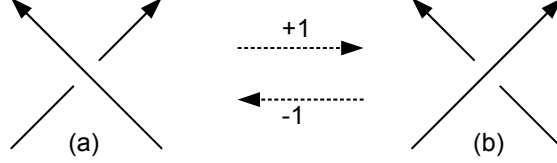


FIGURE 3. Changing a left-handed crossing (a) into a right-handed crossing (b) is denoted by $+1$; the reverse is denoted by -1 .

For each pair of disjoint cycles C_i and C_j in G , denote the linking number of C_i with C_j in Γ_0 and Γ by $\text{lk}(C_i, C_j, \Gamma_0)$ and $\text{lk}(C_i, C_j, \Gamma)$, respectively. Then

$$\text{lk}(C_i, C_j, \Gamma) = \text{lk}(C_i, C_j, \Gamma_0) + \sum_{e_k \in C_i, e_l \in C_j} x_{kl}$$

It follows that G has a D_4 -less embedding Γ iff for each quad (C_1, C_2, C_3, C_4) , at least one of the following equations is satisfied:

$$(1) \quad \text{lk}(C_1, C_3, \Gamma_0) + \sum_{e_k \in C_1, e_l \in C_3} x_{kl} = 0$$

or

$$(2) \quad \text{lk}(C_2, C_4, \Gamma_0) + \sum_{e_k \in C_2, e_l \in C_4} x_{kl} = 0$$

where the linking numbers $\text{lk}(C_i, C_{i+2}, \Gamma_0)$ are calculated numerically by the algorithm. Thus, we have:

Proposition. *Suppose a graph G has Q quads. Choosing one of equations (1) and (2) for each quad gives 2^Q systems of linear equations, with each system consisting of Q equations, such that G has a D_4 -less embedding (in \mathbb{Z} or \mathbb{Z}_2) iff at least one of these systems of equations has a solution (in \mathbb{Z} or \mathbb{Z}_2 , resp.).*

Hence, if G has no D_4 -less embedding, the algorithm would *a priori* need to check every one of these 2^Q systems of equations to reach that conclusion. For the graphs we worked with, the number Q of quads typically ranged from a few thousand to hundreds of thousands, making 2^Q much too large to allow this algorithm to be of practical use. Before we describe the shortcuts we used to speed up the algorithm, we discuss two more issues: (i) integer solutions versus \mathbb{Z}_2 solutions, and (ii) what the solutions to the equations tell us.

Solving a system of equations in \mathbb{Z} , as opposed to in \mathbb{Z}_2 or in \mathbb{R} , requires different methods and can be much slower. So our algorithm first tries to solve each system of equations in \mathbb{Z}_2 . If there is no solution in \mathbb{Z}_2 , we know that there is no solution in \mathbb{Z} either; so the algorithm moves on to the “next” system of equations. However, if a system of equations turns out to have a solution in \mathbb{Z}_2 , then the algorithm determines whether the system also has a solution in \mathbb{R} . If it does, and this solution happens to be in \mathbb{Z} , the algorithm outputs this integer solution and reports that

G has a D_4 -less embedding in \mathbb{Z} . If the system has no real solution or if a real solution is found that is not in \mathbb{Z} , the algorithm moves on to the “next” system of equations. In the end, if no \mathbb{Z}_2 solutions were found for any of the systems, the algorithm reports that the graph is IK. If at least one \mathbb{Z}_2 solution was found but never any integer solutions (we do not recall coming across such a case in our trials), we only conclude that G has a D_4 -less embedding in \mathbb{Z}_2 , (although it may also have one in \mathbb{Z}).

Now let us discuss the case when the algorithm finds an integer solution for one of the systems of equations. This solution tells us how many crossing changes to make between each pair of nonadjacent edges in order to go from Γ_0 to a D_4 -less embedding Γ . These crossing changes can be implemented in different orders and different ways up to isotopy, thus yielding different embeddings of G (Figure 4). And all of these embeddings will be D_4 -less since linking numbers depend only on the total numbers of crossings between nonadjacent pairs of edges. Of course, some or all of these D_4 -less embeddings might contain nontrivial knots. However, every time we tried to, we succeeded in manually finding a knotless embedding by using these prescribed crossing changes as a “rough guide”. Our manual process was by no means algorithmic; it involved making choices in how to implement each crossing change. Making successful choices depended on both experience and luck!

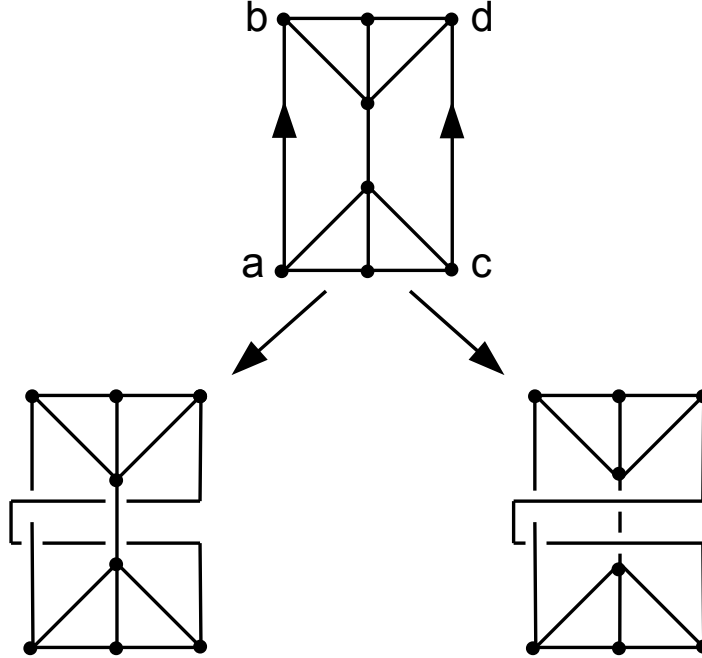


FIGURE 4. Two different ways (among infinitely many) that a “+1 crossing change” (i.e., a full positive twist) can be introduced between the oriented edges ab and cd .

3. THE SHORTCUTS

All of the work in this section applies to both \mathbb{Z} and \mathbb{Z}_2 . With this understood, we will stop repeatedly saying “in \mathbb{Z} or \mathbb{Z}_2 ”.

Let G be a graph. For each quad $q = (C_1, C_2, C_3, C_4)$ in G , let $q(1, 3)$ and $q(2, 4)$ denote the equations one gets in terms of the variables x_{ij} by setting each of $\text{lk}(C_1, C_3)$ and $\text{lk}(C_2, C_4)$, respectively, equal to zero. Let EQ be the set of all equations one obtains in this way from all quads in G , i.e.,

$$EQ = \{q(i, i+2) : i = 1, 2, q \text{ is a quad in } G\}$$

Note that each equation $A \in EQ$ may come from more than one quad. Let's say two equations $A, B \in EQ$ are **related** if there is a quad q such that $\{A, B\} = \{q(1, 3), q(2, 4)\}$. Then, in any D_4 -less embedding of G , at least one equation in each pair of related equations must be satisfied.

One of our shortcuts is as follows. For each equation $A \in EQ$, we find the set $R(A)$ of all equations that are related to A . (Note that by definition $A \notin R(A)$.) In each D_4 -less embedding of G , either A is satisfied or every equation in $R(A)$ is satisfied. So if $R(A)$, considered as a system of equations, has no solution, then A must be satisfied in every D_4 -less embedding of G ; in this case we label A as an **indispensable** equation. We check each equation in EQ for whether it is indispensable, and each time we find a new one, we add it to the collection of all indispensable equations found so far and then check whether this new collection, considered as a system of equations, has a solution. If the collection has no solution, we conclude that G has no D_4 -less embedding, and the algorithm stops. Even when the collection does have a solution, this shortcut can still greatly speed up the algorithm in either finding a D_4 -less embedding or determining that there is none: from among the 2^Q systems of equations, we work only on those systems that contain all the indispensable equations.

Remark: Among the graphs that we worked with, we came across graphs G of both of the following types: (1) G has no D_4 -less embedding but its indispensable equations are satisfiable as a system; (2) G has no D_4 -less embedding and its indispensable equations are not satisfiable as a system.

The second shortcut that we used in the algorithm is as follows. Let $EQ = \{A_1, \dots, A_z\}$ (where the number of equations, z , is at most twice the number quads). We represent each of the 2^Q systems of equations by a string S of 0s and 1s of length z , where the i th digit of S is 1 or 0 according to whether A_i is or is not in the given system of equations.

Of course we are not interested in all strings of 0s and 1s of length z ; we say such a string is **valid** if for each pair of related equations A_i, A_j , the i th or j th digit of S is 1. The algorithm progresses through the set of all valid strings of 0s and 1s of length z from smallest to largest in lexicographical order. The shortcut consists of trying to skip over collections of consecutive strings each of which is either not valid or corresponds to a system of equations that can be predicted, as described below, to have no solution.

Suppose we test and determine a system of equations to have no solution. Often, the rows of the coefficient matrix of such a system turn out to be linearly dependent. We find a linearly independent subset of the rows that span the row space. This corresponds to a subsystem of equations that still has no solution. Thus, any string, valid or not, that contains 1s corresponding to this subsystem should be skipped.

This allows the algorithm to speed up greatly by skipping over large numbers of strings.

We now describe the third shortcut we use in the algorithm. Let C be a cycle in a graph G , and suppose there exist vertices v, w in C such that the edge vw is in G but not in C . Then we say the edge vw is a **chord** for C . If C has no chords, we say it is **chordless**. A quad is said to be chordless if all of its four cycles are chordless. The shortcut is to only find and work with chordless quads instead of all quads. Obviously, if a graph G has a double-linked chordless quad in every embedding, then G is IK. However, a spatial graph that contains a double-linked quad may *a priori* contain no double-linked chordless quad. So an embedding that has no double-linked chordless quads may not be a D_4 -less embedding. It appears though that such cases are rare; in every instance that our algorithm found an embedded graph with no double-linked chordless quads, whenever we tried to we succeeded in manually finding a knotless (and, hence, D_4 -less) embedding for that graph.

4. PROOFS OF THE LEMMAS

Suppose H is a minor of a graph G , with a given sequence S of edge contractions that turn a subgraph G' of G into H . We say a path p' in $G' \subset G$ **corresponds** to a path p in H if the given sequence S of edge contractions turns p' into p . (Note that a path may be a cycle or just one vertex.) There may be different subgraphs G' of G with different sequences S of edge contractions through which one can obtain H as a minor of G ; and correspondence between two paths certainly depends on the choice of G' and S . So whenever we say p' corresponds to p , it is to be understood that the correspondence is relative to the given G' and S .

When working with simple graphs, i.e., graphs with no loops or double edges, it is a common convention that whenever an edge contraction results in a double edge, the two edges in the resulting double edge are “merged together” into one edge. However, in this paper we work with D_4 , which is a multigraph; hence we do *not* adopt this convention. In other words, we do allow loops, and we do not merge together double edges. An advantage of this is that if H is obtained from a subgraph of a graph G by a finite sequence of edge contractions, then clearly *to each edge in H there corresponds a unique edge in G* . As we will see in Lemma 1 below (which is used to prove Lemma 2), the same is true for cycles (though not necessarily for all paths).

Lemma 1. *Suppose H is obtained from a subgraph of a graph G by a given sequence of edge contractions, where double edges are not merged together and loops are not deleted. Then to every cycle C in H there corresponds a unique cycle C' in G .*

Proof. We use induction on the number of contracted edges. Suppose H is obtained from a subgraph G' of G by contracting one edge e_0 in G' . For each edge e in H , let e' denote the unique edge in G' that corresponds to e . Let C be a cycle in H . Let $E(C)$ denote the set of edges in C . Then exactly one of $\bigcup_{e \in E(C)} e'$ or $\bigcup_{e \in E(C)} e' \cup \{e_0\}$ is a cycle in $G' \subseteq G$; and this cycle becomes C after we contract e_0 . The lemma now follows by induction. \square

Lemma 2. *If a spatial graph Γ contains a double-linked D_4 (in \mathbb{Z} or \mathbb{Z}_2) as a minor, then it contains a double-linked quad (in \mathbb{Z} or \mathbb{Z}_2 , respectively).*

Proof. We use induction on the number of contracted edges. To prove the “base case”, we simply note that a double-linked D_4 clearly contains a double-linked quad.

As our induction hypothesis, assume Ω is a spatial graph that contains a double-linked quad and is obtained from Γ by contracting one edge $e_0 \subset \Gamma$ into a vertex $v_0 \in \Omega$. We will show Γ contains a double-linked quad.

Let (C_1, C_2, C_3, C_4) be a double-linked quad in Ω with connecting paths p_1, \dots, p_4 . By Lemma 1, there exist unique cycles C'_1, \dots, C'_4 in Γ that correspond to C_1, \dots, C_4 . It is easy to check that $\text{lk}(C'_i, C'_{i+1}) = \text{lk}(C_i, C_{i+1})$ (in \mathbb{Z} or \mathbb{Z}_2). We now construct connecting paths q_1, \dots, q_4 for (C'_1, \dots, C'_4) . (We use q_i instead of p'_i to denote these paths because some of them may not correspond to the p_i .) Fix $i \in \{1, 2, 3, 4\}$. We have two cases.

Case 1. $C_i \cap C_{i+1}$ is nonempty and connected. Then one verifies easily that $C'_i \cap C'_{i+1}$ too is nonempty and connected. So we let q_i be any vertex in $C'_i \cap C'_{i+1}$.

Case 2. $C_i \cap C_{i+1} = \emptyset$. We have two subcases:

- (a) v_0 is not in p_i , or v_0 is in the interior of p_i . Then, by an argument similar to the proof of Lemma 1, there is a unique path in Γ that corresponds to p_i . We let q_i be this path.
- (b) v_0 is in p_i and v_0 is not in the interior of p_i . Hence v_0 is an endpoint of p_i and must lie in exactly one of C_i or C_{i+1} . Without loss of generality, assume $v_0 \in C_i$. Let p'_i be the path whose edges correspond to the edges of p_i . If p'_i has an endpoint in C'_i , we let $q_i = p'_i$; otherwise we let $q_i = p'_i \cup \{e_0\}$.

Now it is not difficult to see that (C'_1, C'_2, C'_3, C'_4) and q_1, \dots, q_4 satisfy the definition of a double-linked quad in Γ . \square

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